OptiDis: Toward fast anisotropic dislocation dynamics based on Stroh formalism

Pierre Blanchard, Arnaud Etcheverry, Olivier Coulaud, Laurent Dupuy, Marc Bletry

OptiDis: Toward fast anisotropic DD based on Stroh formalism.

Pierre Blanchard[1] - Arnaud Etcheverry [1] - Olivier Coulaud [1] - Laurent Dupuy [2] - Marc Blétry [2]

[1]: HiePACS team project, Inria Bordeaux - Sud-Ouest, 200, rue Vieille Tour 33405 Talence Cedex France | [2]: Service de Recherches Métallurgiques Appliquées, CEA-Saclay, 91191 Gif-sur-Yvette, France

ABSTRACT

Dislocation Dynamics (DD) simulations in the hypothesis of isotropic elasticity have proved great reliability in order to predict the plastic behaviour of crystalline materials. However it is often the case at high temperature (for instance in irradiated BCC iron) that the structural properties of a material will be better described using full anisotropic treatment of the elastic interaction between dislocations. The computation of the internal elastic forces is by far the most resources consuming step in DD simulations, which is even more true for anisotropic elasticity in the absence of explicit Green's function.

L. Dupuy, J. Soulacroix and M. Fivel showed that the approaches summarized in Yin [6] can be accelerated using spherical harmonics expansions of the Stroh matrices. This feature was implemented in the DD code OptiDis in order to power the anisotropic forces computation. Here we recall the formalism and we discuss optimizations, performances as well as motivations for future developments.

ANISOTROPIC MODEL

The stress field created by a dislocation loop $(\mathbf{b}', \mathbf{t}')$ at field point $\mathbf{x}$ is given by Mura's formula [4]

$$\sigma_{js}(\mathbf{x}) = \varepsilon_{ngr} C_{jsvg} C_{pqwn} b'_w \oint_C \frac{\partial G_{vp}}{\partial x_q}(\mathbf{x}-\mathbf{x}')dx'_r \qquad (1)$$

The nodal force $\mathbf{f}_n^e$ acting at the extremities of a finite dislocation line $(\mathbf{b}, \mathbf{t})$ is obtained by integration of the Peach-Koehler force $(\mathbf{f}^{PK} = (\boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{b}) \times \mathbf{t}(\mathbf{x}))$ over the target line, i.e.

$$(f_n^e)_\alpha = \oint_{(C)} \varepsilon_{\alpha\beta\gamma} \sigma_{\beta p} b_p t_\gamma N_n(\mathbf{x}) dx$$

where $N_{n=1,2}$ are linear shape functions. The cost of updating the nodal forces at each time step is quadratic and involves the evaluation of 2 line integrals, therefore it is usually the bottleneck of DD simulations. Moreover there does not exist an analytic closed form for the anisotropic elastic Green's function G. Recently Aubry et al. [2] used an integral representation of G and developped a fast method based on spherical harmonic expansions in order to evaluate the double line integral semi-analytically. On the other hand, past works [6] showed that the anisotropic stress field can be efficiently described using the Stroh sextic formalism combined with (2) the Willis-Steeds-Lothe formula for the finite line.

Willis-Steeds-Lothe

$$u_{m,s} = \frac{1}{4\pi d}\varepsilon_{jsn} b_i C_{ijkl} t_n \left\{-m_l Q_{mk} + n_l \left[(nn)^{-1}(nm)Q\right]_{mk} + n_l \left[(nn)^{-1}S^T\right]_{mk}\right\}_{\tau_1}^{\tau_2} \qquad (2)$$

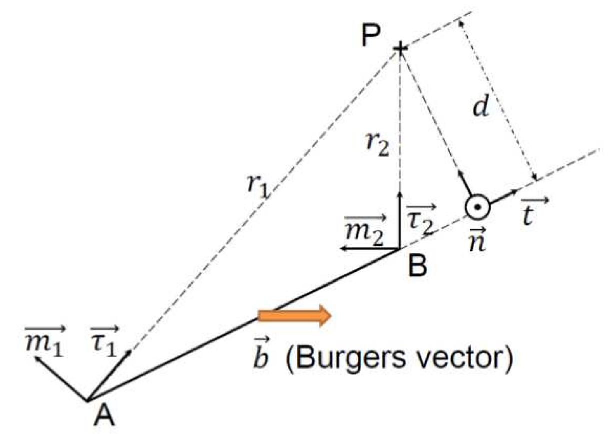

FIGURE 1: Notations for the stress created by segment AB on a field point P.

where Stroh matrices $\mathbf{Q}$ and $\mathbf{S}$ [5] only depend on C_{ijkl} and $\boldsymbol{\tau}$. They are computed from the eigenvectors of a 6×6 matrix $\mathbf{N}$ depending on (nn) and (nm) where $(ab)_{jk} = a_i C_{ijkl} b_l$. The notations are recalled fig 1 and the stress field reads

$$\sigma_{ij}(\mathbf{x}, \mathbf{t}, \mathbf{b}) = C_{ijkl} u_{k,l}(\mathbf{x}, \mathbf{t}, \mathbf{b})$$

In the collinear case $(d = 0)$ the expression is slightly more complicated but can be condensed as follows

$$u_{m,s}(d = 0) = \left(\frac{1}{r_2} - \frac{1}{r_1}\right)\frac{1}{4\pi} b_i Z_{ims}$$

The singularity in the limit $r \to 0$ is currently handled using a simple cutoff parameter like the one defined in [6].

Anisotropy ratio

The degree of anisotropy is quantified by the ratio $A = 2C_{44}/(C_{11} - C_{12})$. For the BCC $\alpha - Fe$, this ratio goes from $A_{0K} = 2.3$ to $A_{1200K} = 7.1$.

SPHERICAL HARMONIC ANALYSIS

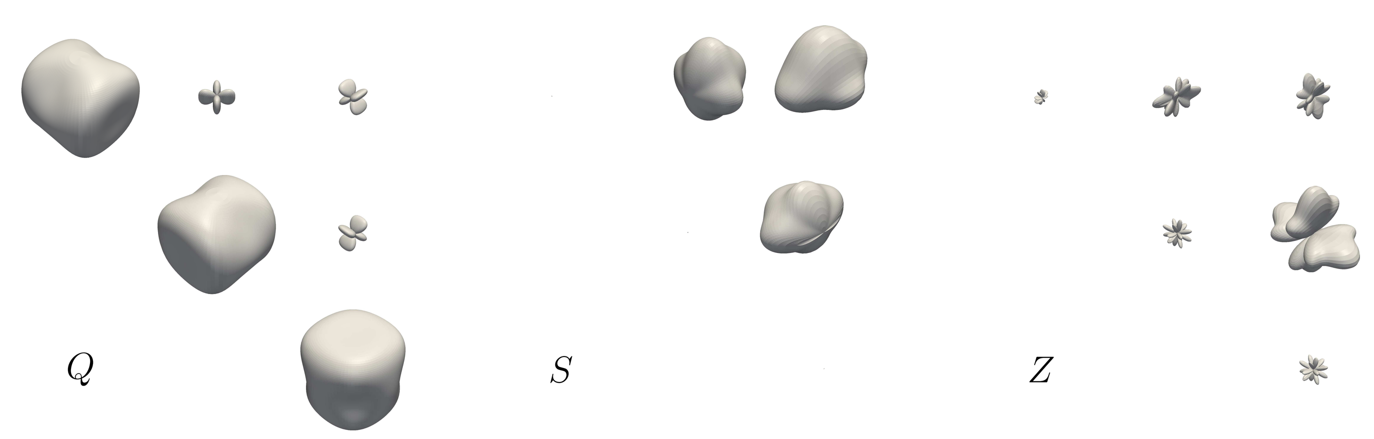

FIGURE 2: Stroh matrices components at $(T = 25°C)$ for $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$.

Spherical harmonic analysis

Stroh matrices only depend on the orientation of the source, i.e. $\mathbf{X} = \mathbf{X}(\theta, \phi)$ (see fig 2) hence they can be expanded into spherical harmonics.

$$\mathbf{X}(\theta, \phi) \approx \sum_{\ell=0}^{\ell_{max}} \sum_{m=-\ell}^{\ell} \mathbf{x}_\ell^m Y_\ell^m(\theta, \phi)$$

where Y_ℓ^m denotes the well known spherical harmonics and

$$\mathbf{x}_\ell^m = \int_0^\pi \int_0^{2\pi} \mathbf{X}(\theta, \phi) Y_\ell^m(\theta, \phi) \sin\theta d\theta d\phi \qquad (3)$$

are the coefficients of the expansion.

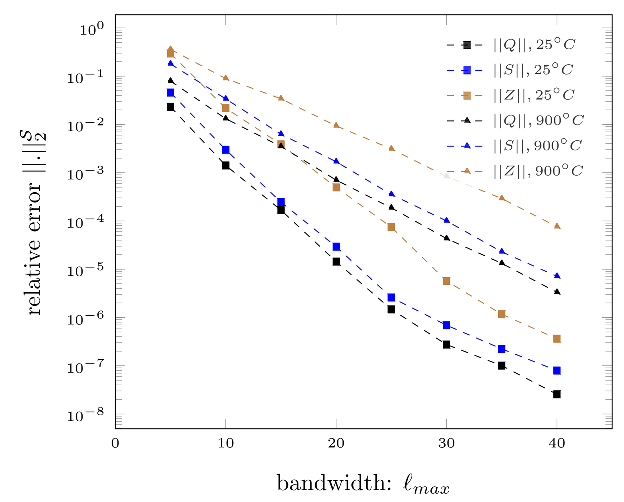

FIGURE 3: Accuracy of the expansion for various temperatures.

Given that Stroh matrices are real valued the expansion reduces to

$$\mathbf{X} \approx \sum_{\ell=0}^{\ell_{max}} \mathbf{x}_\ell^0 Y_\ell^0 + 2\sum_{m=1}^{\ell} Re(\mathbf{x}_\ell^m)Re(Y_\ell^m) - Im(\mathbf{x}_\ell^m)Im(Y_\ell^m)$$

On the other hand depending on the symmetries of $\mathbf{X}$ in θ or ϕ some coefficients of the expansions are known to be null (potentially a lot). Once implemented these simplifications lead to a significant acceleration of the method (see fig 4).

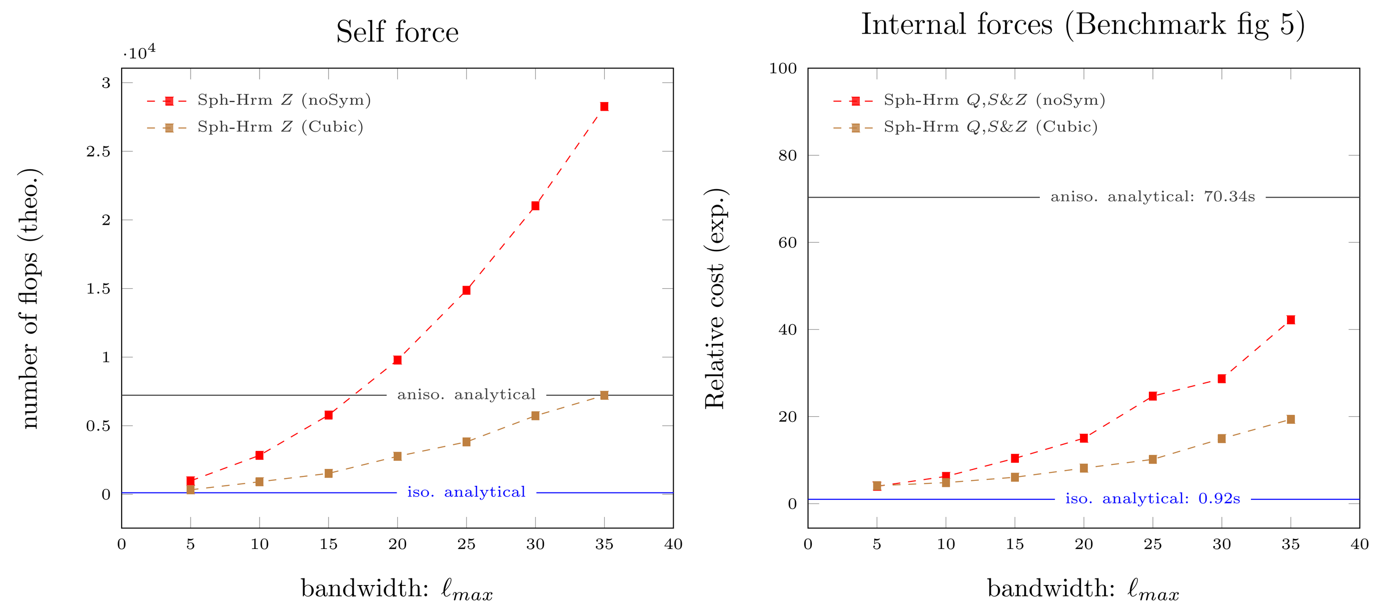

FIGURE 4: Theoretical number of flops involved in self force evaluation (left) and relative computational cost for ≈ 3000 segments based on CPU time (right).

The precomputation of the 2 integrals (3) is done exactly following the method described by Driscoll and Healy [3], namely using an equispaced quadrature in ϕ and a gaussian quadrature in $\cos\theta$.

IMPLEMENTATION AND PERFORMANCES

Our experimentations were performed on the core program OptiDis whose data structure relies heavily on the open source ScalFMM library [1]. The latter also provides the generic Fast Multipole algorithms. OptiDis is a parallel version of NumoDis, it implements almost all functionalities of NumoDis while providing a hybrid OpenMP/MPI paradigm and a cache-conscious data structure.

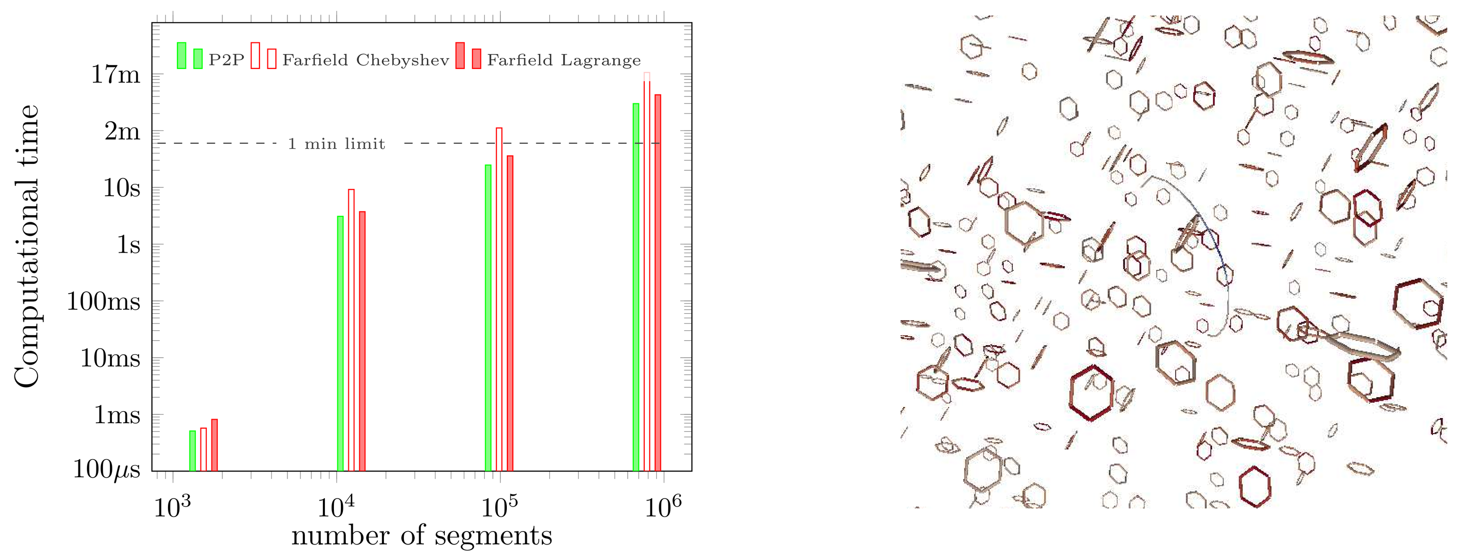

FIGURE 5: Isotropic near- and farfield computational time balancing for a uniform distribution of dislocation loops and increasing tree depth (left). An example of defects distribution and a propagating Frank-Read source (right).

ONGOING & PERSPECTIVES

Ongoing

- Optimized expansion for hexagonal crystallographies

Perspectives

- Implementation of the farfield (either iso- or anisotropic)
- Efficient analytic integration of the expansion over the target segments
- Derivation of a consistent non-singular theory for the Stroh approach

REFERENCES

[1] Scalfmm: software library to simulate large scale n-body interactions using the fast multipole method, developped @ hiepacs team, inria bordeaux.

[2] S Aubry and A Arsenlis. Use of spherical harmonics for dislocation dynamics in anisotropic elastic media. *Modelling and Simulation in Materials Science and Engineering*, 21(6):065013, 2013.

[3] James R Driscoll and Dennis M Healy. Computing fourier transforms and convolutions on the 2-sphere. *Advances in applied mathematics*, 15(2):202–250, 1994.

[4] Toshio Mura. *Micro-mechanics of Defects in Solids*, volume 3. Springer, 1987.

[5] AN Stroh. Steady state problems in anisotropic elasticity. *J. math. Phys*, 41(2):77–103, 1962.

[6] Jie Yin, David M Barnett, and Wei Cai. Efficient computation of forces on dislocation segments in anisotropic elasticity. *Modelling and Simulation in Materials Science and Engineering*, 18(4):045013, 2010.

FUNDINGS

This work was supported by the French ANR grants ANR-10-COSI-0011 and the associate team FastLA.

In collaboration with CEA Saclay | More videos & infos →